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Truck Transport of Hazardous Chemicals: Phosphorus Pentasulfide

Final Report
August 1996

U.S. Department of Transportation
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Cambridge, MA 02142-1093

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The transport of hazardous materials by all modes is a major concern of the U.S. Department of Transportation. Estimates place the total amount of hazardous materials transported in the United States in excess of 1.5 billion tons per year. Highway, water, and rail account for nearly all hazardous materials shipments; air shipments are negligible. Fuels, such as gasoline and diesel, account for about half of all hazardous materials transported. Chemicals account for most of the remainder.

The principal purpose of this report is to present estimates of truck shipments of phosphorus pentasulfide, one of 147 large-volume chemicals that account for at least 80 percent of U.S. truck shipments of hazardous chemicals.

All of the reports in this series are based on the best available information at the time the research was conducted. The U.S. chemical industry, however, operates in an environment in which markets, production processes, and distribution requirements can change substantially from year to year. The information in this report on (a) chemical producers and their plant locations, (b) consuming plants and their locations, and (c) the estimated traffic flow from producers to consumers, is thus subject to change.

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PREFACE

The transport of hazardous materials by all modes is a major concern of the U.S. Department of Transportation (U.S. DOT). Estimates place the total amount of hazardous materials transported in the United States in excess of 1.5 billion tons per year.[1] Highways, water, and rail account for nearly all hazardous materials shipments; air shipments are negligible. Fuels, such as gasoline and diesel, account for about half of all hazardous materials transported. Chemicals account for most of the remainder.

Because of the intermixture of freight and passenger vehicles on the Nation's roads and highways, and because hazardous materials are frequently transported through residential and commercial areas, incidents involving truck movements of hazardous materials may pose a risk to the general population. The U.S. DOT has extensive data on highway incidents involving particular hazardous materials, but does not have comparable volume data with which to establish failure rates (i.e., the percentage of shipments involved in incidents). Moreover, little is known about the routes over which particular hazardous materials are transported. Consequently, Federal and state authorities lack critical information they need to formulate hazardous materials policies and programs regarding enforcement of regulations, training for dealing with hazardous materials incidents, etc.

This document is one of a series of reports being prepared on the transport of large-volume manufactured or processed non-fuel substances that together account for at least 80 percent of U.S. truck shipments of hazardous chemicals. It was sponsored by the Office of Hazardous Materials Safety, Research and Special Programs Administration (RSPA), U.S. DOT. The report was prepared by the Environmental Engineering Division, Volpe National Transportation Systems Center, U.S. DOT, and TDS Economics, Menlo Park, California.

It should be emphasized that all of the reports in this series are based on the best available information at the time the research was conducted. The U.S. chemical industry, however, operates in a dynamic economic and technological environment in which markets, production processes, and distribution requirements can change substantially from year to year. The information in this report on (a) chemical producers and their plant locations, (b) consuming plants and their locations, and (c) the estimated traffic flows from producers to consumers is thus subject to change.

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[1] Office of Technology Assessment, Congress of the United States, *Transportation of Hazardous Materials*, 1986 and Research and Special Programs Administration, U.S. Department of Transportation, *Truck Transportation of Hazardous Materials, A National Overview,* 1987.

METRIC/ENGLISH CONVERSION FACTORS

ENGLISH TO METRIC

LENGTH (APPROXIMATE)

1 inch (in) = 2.5 centimeters (cm)
1 foot (ft) = 30 centimeters (cm)
1 yard (yd) = 0.9 meter (m)
1 mile (mi) = 1.6 kilometers (km)

AREA (APPROXIMATE)

1 square inch (sq in, in^2) = 6.5 square centimeters (cm^2)
1 square foot (sq ft, ft^2) = 0.09 square meter (m^2)
1 square yard (sq yd, yd^2) = 0.8 square meter (m^2)
1 square mile (sq mi, mi^2) = 2.6 square kilometers (km^2)
1 acre = 0.4 hectare (ha) = 4,000 square meters (m^2)

MASS - WEIGHT (APPROXIMATE)

1 ounce (oz) = 28 grams (gm)
1 pound (lb) = .45 kilogram (kg)
1 short ton = 2,000 pounds (lb) = 0.9 tonne (t)

VOLUME (APPROXIMATE)

1 teaspoon (tsp) = 5 milliliters (ml)
1 tablespoon (tbsp) = 15 milliliters (ml)
1 fluid ounce (fl oz) = 30 milliliters (ml)
1 cup (c) = 0.24 liter (l)
1 pint (pt) = 0.47 liter (l)
1 quart (qt) = 0.96 liter (l)
1 gallon (gal) = 3.8 liters (l)
1 cubic foot (cu ft, ft^3) = 0.03 cubic meter (m^3)
1 cubic yard (cu yd, yd^3) = 0.76 cubic meter (m^3)

TEMPERATURE (EXACT)

°C=5/9(°F - 32)

METRIC TO ENGLISH

LENGTH (APPROXIMATE)

1 millimeter (mm) = 0.04 inch (in)
1 centimeter (cm) = 0.4 inch (in)
1 meter (m) = 3.3 feet (ft)
1 meter (m) = 1.1 yards (yd)
1 kilometer (km) = 0.6 mile (mi)

AREA (APPROXIMATE)

1 square centimeter (cm^2) = 0.16 square inch (sq in, in^2)
1 square meter (m^2) = 1.2 square yards (sq yd, yd^2)
1 square kilometer (km^2) = 0.4 square mile (sq mi, mi^2)
10,000 square meters (m^2) = 1 hectare (ha) = 2.5 acres

MASS - WEIGHT (APPROXIMATE)

1 gram (gm) = 0.036 ounce (oz)
1 kilogram (kg) = 2.2 pounds (lb)
1 tonne (t) = 1,000 kilograms (kg) = 1.1 short tons

VOLUME (APPROXIMATE)

1 milliliter (ml) = 0.03 fluid ounce (fl oz)
1 liter (l) = 2.1 pints (pt)
1 liter (l) = 1.06 quarts (qt)
1 liter (l) = 0.26 gallon (gal)
1 cubic meter (m^3) = 36 cubic feet (cu ft, ft^3)
1 cubic meter (m^3) = 1.3 cubic yards (cu yd, yd^3)

TEMPERATURE (EXACT)

°F=9/5(°C) + 32

QUICK INCH-CENTIMETER LENGTH CONVERSION

INCHES	0			1			2		3		4			5
CENTIMETERS	0	1	2	3	4	5	6	7	8	9	10	11	12	13

QUICK FAHRENHEIT-CELSIUS TEMPERATURE CONVERSION

°F	-40°	-22°	-4°	14°	32°	50°	68°	86°	104°	122°	140°	158°	176°	194°	212°
°C	-40°	-30°	-20°	-10°	0°	10°	20°	30°	40°	50°	60°	70°	80°	90°	100°

For more exact and or other conversion factors, see NIST Miscellaneous Publication 286, Units of Weights and Measures. Price $2.50. SD Catalog No. C13 10286.

Updated 8/1/96

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1. INTRODUCTION

The principal purpose of this report is to present estimates of truck shipments of phosphorus pentasulfide, one of the 147 large-volume chemicals that account for at least 80 percent of U.S. truck shipments of hazardous chemicals. Appendix A lists these chemicals and their estimated 1987 production volumes.

The following sections of this report describe the physical characteristics of phosphorus pentasulfide, its uses, and domestic producers and users. Because there is so little direct evidence on the specific routes over which phosphorus pentasulfide is shipped, and in what quantities, this information is estimated by the use of models. Two widely-used models of interregional commodity flows have been used: a gravity model and a linear programming model, each generating its own set of results. Both sets of results show quantities of phosphorus pentasulfide flowing through individual states, and both are displayed graphically on flow maps.

Unfortunately, there are insufficient data on actual flows of phosphorus pentasulfide to test model results for accuracy or to determine which model provides the more reliable estimates. It is shown, however, that the results of at least one of the models is consistent with RSPA data on incidents involving truck shipments of phosphorus pentasulfide. More importantly, although the results of the two models are somewhat different, they agree in their identification of the major routes that carry phosphorus pentasulfide, which is a major objective of this research.

2. CHARACTERISTICS OF PHOSPHORUS PENTASULFIDE

Phosphorus pentasulfide is a high melting point solid. It is flammable, produces poisonous, irritating gases when ignited, can irritate the skin and eyes in case of exposure, and is harmful if swallowed. The *1996 North American Emergency Response Guidebook* recommends that emergency responders use its Guide No. 139 (UN 1340) in the case of a phosphorus pentasulfide spill. Additional information about phosphorus pentasulfide is given in Table 1.

3. USES OF PHOSPHORUS PENTASULFIDE

Phosphorus pentasulfide is used primarily in the production of pesticides and lubricating oil additives. It is also used in the production of industrial surfactants and water treatment compounds, including heavy duty detergents, waterless hand cleaners, and mold release agents.

TABLE 1. ADDITIONAL INFORMATION ON PHOSPHORUS PENTASULFIDE

Common Synonyms	Phosphoric sulfide Phosphorus persulfide Phosphorus sulfide Thiophosphoric anhydride Sulfur phosphide
Formula	P_2S_5
UN Number	1340
DOT Hazard Class/Division	4.3 (Dangerous when wet materials)
CAS Number	1314-80-3
Description	Solid flakes or powder Yellow to green Odorless or rotten egg odor

Sources: *CHRIS Manual, Vol. 1, Condensed Guide to Chemical Hazards*, 1992; National Tank Truck Carriers, Inc., *Hazardous Commodity Handbook*, Tenth Edition, 1994; and Gale Research, Inc., *Hazardous Substances Resource Guide*, 1993.

4. PRODUCTION

Production of phosphorus pentasulfide takes place in four plants located in the East and Midwest. With an estimated U.S. production of 70 thousand short tons in 1987, this chemical is in the lower third of the list of chemicals in Appendix A. The chemicals listed in that appendix account for over 80 percent (by volume) of truckload shipments of hazardous chemicals in the United States.

Phosphorus pentasulfide is frequently used in the manufacture of other chemicals at its producing plants. Intraplant use is termed "captive production." To calculate captive production, downstream chemicals produced within the same plant are identified, and the amount of phosphorus pentasulfide needed in their production is estimated. The difference between total production capacity and captive production defines the amount available for off-site shipments. It is the amount of production available for off-site consumption that is of interest to this study.

Table 2 shows net production available for off-site consumption by producing plant.

TABLE 2. MAJOR PRODUCERS OF PHOSPHORUS PENTASULFIDE, 1987

Company	Plant Location	ZIP Code	Off-site Availability† (Thousands of Short Tons)
FMC	Lawrence, KS	66044	18.0
ICI	Mount Pleasant, TN	38474	0.6
Monsanto	Sauget, IL	62201	27.0
Rhone-Poulenc	Morrisville, PA	19067	19.0
Total Off-site Availability			64.6

†Shipments available for off-site sales, or total production capacity less captive production.

Sources: SRI International, *Study of Truck Transportation of Hazardous Chemicals*, SRI Project 8511, prepared for U.S. DOT, March 1993, and industry contacts.

5. CONSUMPTION

Twelve plants, all located in the Mid-Atlantic, Great Lakes, and Southern states, are identified as net consumers of phosphorus pentasulfide. One of the consuming plants does not receive shipments by truck. The remaining eleven sites are listed in Table 3, along with their net product requirements for phosphorus pentasulfide. Note that 1987 net product requirements of 44.3 thousand short tons were less than the total off-site availability of 64.6 thousand short tons. That is, the producing plants had the capacity to manufacture more than the consuming plants required in 1987.

TABLE 3. MAJOR CONSUMERS OF PHOSPHORUS PENTASULFIDE THAT RECEIVE SHIPMENTS BY TRUCK, 1987

Company	Plant Location	ZIP Code	Estimated Net Product Requirement (Thousands of Short Tons)
Consumers Receiving Shipments by Truck			
American Cyanamid	Hannibal, MO	63401	4.5
American Cyanamid	Linden, NJ	07036	4.3
Amoco	Wood River, IL	62095	2.3
Chevron	Belle Chasse, LA	70037	3.1
Elco	Hooven, OH	45033	0.3
Ethyl	Sauget, IL	62201	3.6
FMC†	Baltimore, MD	21226	0.6
ICI†	Cold Creek, AL	36512	0.6
Lubrizol	Painesville, OH	44077	6.8
Mobay	Kansas City, MO	64120	7.4
Texaco	Port Arthur, TX	77640	3.9
Total Truck Shipments			37.4
Total Rail Shipments			6.9
Total Shipments, All Modes			44.3

†Captive consuming plants, or plants owned by the same parent as one or more of the producing plants.

Sources: SRI International, *Study of Truck Transportation of Hazardous Chemicals*, SRI Project 8511, prepared for U.S. DOT, March 1993, and U.S. Department of Transportation, HMIS database.

6. DISTRIBUTION AND TRANSPORT

Interviews with consumers of phosphorus pentasulfide indicate that shipments move by rail and truck, but not by water. It is carried in fiber or steel drums and tote bins. There are also bulk shipments in specially constructed tank trucks.

According to research conducted for this study, about 88 percent (by weight) of the shipments of phosphorus pentasulfide move by truck. One possible reason for heavy reliance on truck transportation may be the extremely hazardous nature of this chemical, which would encourage the use of many small shipments rather than a few large shipments.

The interviews with consumers also yielded information useful to the modeling of truck transport, discussed in the next section. For example, ICI, one of the four producers, does not sell any of its phosphorus pentasulfide available for off-site shipments on the merchant market, but does ship the product from its plant in Mount Pleasant, Tennessee, to the ICI plant in Cold Creek, Alabama.

7. USE OF MODELS TO ESTIMATE TRUCK FLOWS

This section explains how the producer and consumer information in Tables 2 and 3 is used to identify the specific highways over which bulk shipments of phosphorus pentasulfide are transported from producers to users and in what quantities.

Because there is so little readily available direct evidence on the flows of phosphorus pentasulfide over the Nation's highways, those flows must be estimated. For this report, this was accomplished by the use of two widely used models of interregional commodity flows, a gravity model and a linear programming model. Using the data in Tables 2 and 3, both models allocate truck flows from the producing plants to consuming plants. The basic features of these models are described in Appendix B.[2]

Both models have been adjusted to take into account some real-world features of the distribution of hazardous chemicals:

- Some shipments are made to captive consumers, that is, to consuming plants owned by the same parent company as the producing plant.

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[2]A more detailed, technical explanation of the models is found in "Alternative Modeling Approaches for Allocating Truck Flows of Hazardous Chemicals," a draft report prepared for RSPA's Office of Hazardous Materials Safety by the RSPA/Volpe Center and TDS Economics, July 1994.

- As a matter of company policy, some consuming plants do not purchase from certain producers.

- Regulations mandate the use of two drivers for trips that are over 230 miles in length.

There appears to be no consensus as to which model provides the more accurate estimates of routes used for truck shipments of hazardous chemicals. The gravity model, however, may well have identified some flows of phosphorus pentasulfide that do not in fact exist. For example, according to the gravity model results (See Figures 3 and 4 in Appendix C), there is a major flow of phosphorus pentasulfide from the Monsanto plant in Sauget, Illinois to the Lubrizol plant in Painesville, Ohio, despite the fact that the Lubrizol plant should be able to obtain all of the phosphorus pentasulfide it needs from nearby Morrisville, Pennsylvania. Also unlikely are the long shipments through Tennessee and Virginia to consuming plants for which there are closer potential sources of supply. A number of other, smaller flows appear to be inconsistent with efficient truck distribution of phosphorus pentasulfide. Given the locations of the producing and consuming plants, the results of the linear programming model appear to be more consistent with the minimization of ton-miles, and thereby of the cost of shipping phosphorus pentasulfide. These results are presented in the main body of the report, and the results of the gravity model are presented in an appendix. A key point to be emphasized, however, is that the two models do agree on at least some of the major truck routes that carry phosphorus pentasulfide.

8. LINEAR PROGRAMMING MODEL ESTIMATION RESULTS

The linear programming results for bulk shipments of phosphorus pentasulfide are shown in Table 4.[3] Of the estimated 5.2 million ton-miles of phosphorus pentasulfide moved by truck in 1987, 18 percent occurred in Oklahoma and 17.5 percent occurred in Mississippi, neither of which has plants that either produce or consume phosphorus pentasulfide. Shipments from the Rhone-Poulenc plant in Morrisville, Pennsylvania, northwest to Painesville, Ohio, and east to Linden, New Jersey, and to Baltimore, Maryland account for the 13 percent that occurred in Pennsylvania. Twelve percent of the ton-miles flowed through Texas, which carried the traffic from Lawrence, Kansas, to Port Arthur, Texas.

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[3]The gravity model results are shown in Appendix C.

TABLE 4. LINEAR PROGRAMMING ESTIMATES OF BULK TRUCK SHIPMENTS OF PHOSPHORUS PENTASULFIDE BY STATE, 1987

State	Ton-miles (Thousands)	Truck-miles (Thousands)†
Alabama	210	8
Arkansas	224	8
Delaware	14	1
Illinois	164	6
Indiana	46	2
Kansas	105	4
Louisiana	310	11
Maryland	36	1
Mississippi	908	33
Missouri	264	10
New Jersey	196	7
Ohio	412	15
Oklahoma	936	34
Pennsylvania	670	24
Tennessee	76	3
Texas	621	23
Total	5,192	189

†The short tons per vehicle range from 15 to 40, including both flat beds and containers. Truck-miles are calculated by dividing ton-miles by 27.5, the mid-point of this range.

The linear programming model results shown in Table 4 are reflected on the maps in Figures 1 and 2, which show the major routes carrying truck shipments of phosphorus pentasulfide.[4] The width of the blue lines is directly proportional to the quantity flowing over the routes, as indicated in the figure legends. The direction of flow is indicated by the position of the flow line relative to its route, shown in red. A blue flow line shown to the right of a north-south route indicates that the flow is northward. A blue flow line that lies above an east-west route line indicates that the flow is westward.

Starting with the westernmost flows, phosphorus pentasulfide is shipped from the FMC plant in Lawrence, Kansas, to nearby Kansas City, Missouri. It is also shipped to Port Arthur, Texas, through southeast Kansas, central Oklahoma and northeastern Texas. The Monsanto plant in Sauget, Illinois, ships phosphorus pentasulfide to an Ethyl plant, also in Sauget, Illinois. It also ships to nearby Hannibal, Missouri, and Wood River, Illinois; also east across Illinois and Indiana to Hooven, Ohio. The longest highway shipment from Sauget, Illinois, is that to Belle Chasse, Louisiana, through southeastern Missouri and western Mississippi. A relatively small amount of phosphorus pentasulfide is transported by truck from the ICI plant in Mount Pleasant, Tennessee, down through Alabama to the ICI plant in Cold Creek. The Rhone-Poulenc plant in Morrisville, Pennsylvania, ships phosphorus pentasulfide by truck northwest to the Lubrizol plant in Painesville, Ohio; also east across southern Pennsylvania to the American Cyanamid plant in Linden, New Jersey, and down to the FMC plant in Baltimore, Maryland.

[4]The software used to generate the flow maps is described in Appendix D.

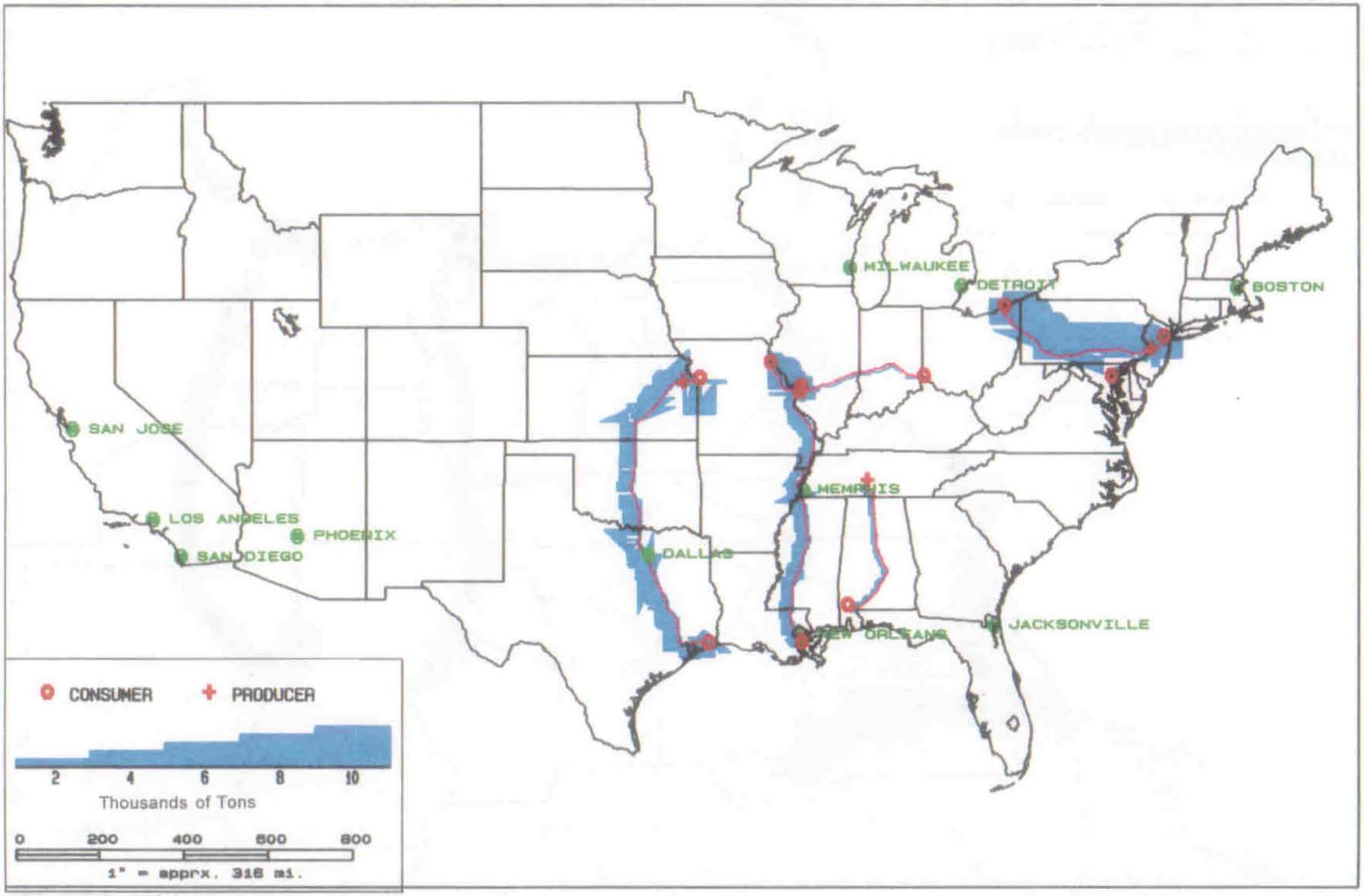

FIGURE 1. NATIONAL TRUCK FLOWS OF PHOSPHORUS PENTASULFIDE
(LINEAR PROGRAMMING RESULTS)

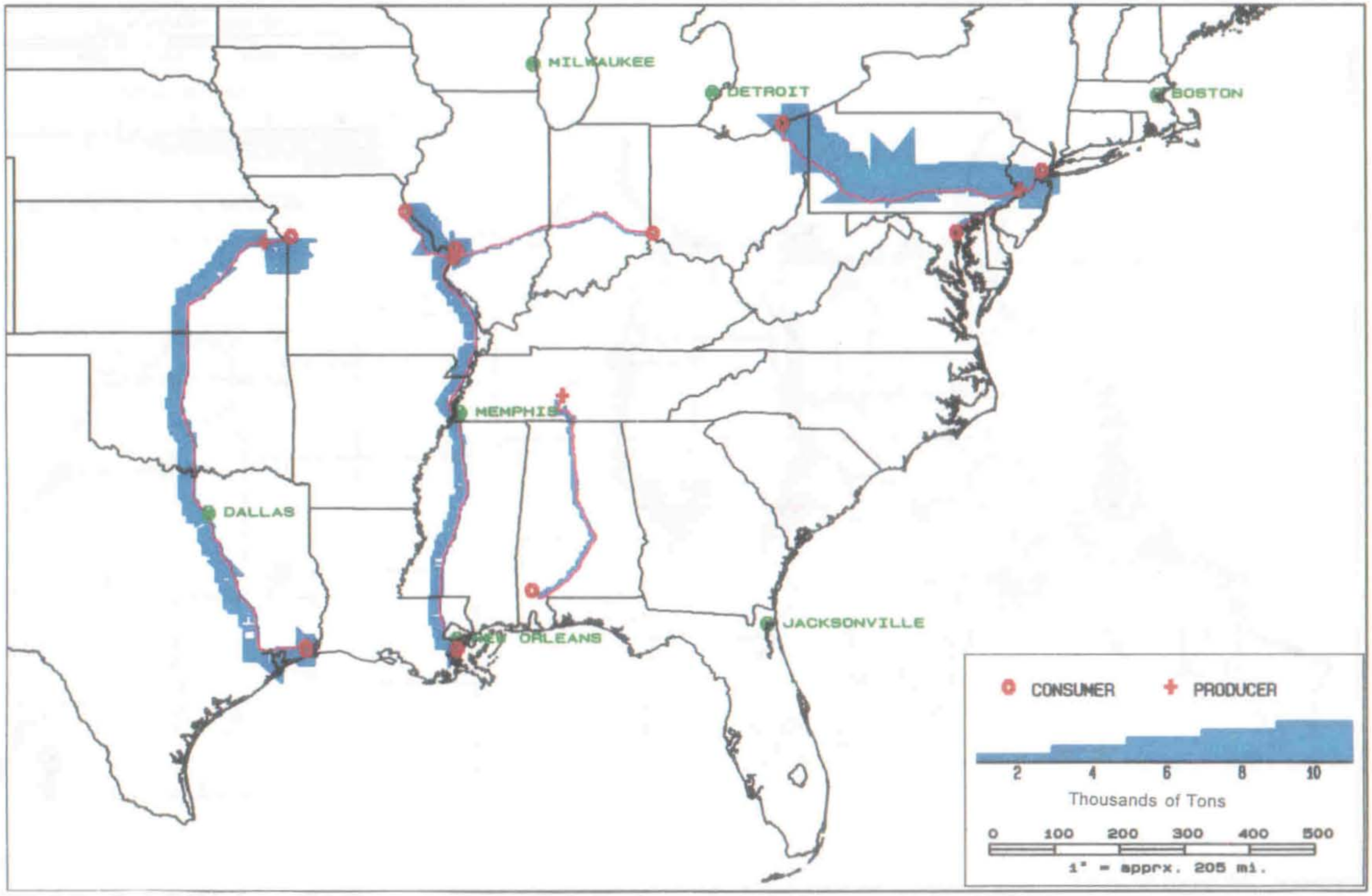

FIGURE 2. NATIONAL TRUCK FLOWS OF PHOSPHORUS PENTASULFIDE: EASTERN U.S. (LINEAR PROGRAMMING RESULTS)

9. COMPARISON OF MODEL RESULTS WITH INCIDENT DATA

Table 5 shows estimates of the expected annual number of truck accidents involving phosphorus pentasulfide. These estimates are based on 1987 truck-miles, shown in Table 4. Given RSPA's estimate that about 15 percent of highway accidents result in a release or spill, the last column shows the expected number of years between spills for each state.

The estimates in Table 5 indicate that, as of 1987, the states with the highest risk of both truck accidents and spills were Mississippi, Ohio, Oklahoma, Pennsylvania, and Texas. This is hardly surprising, since these states also rank highest in ton-miles and truck-miles of phosphorus pentasulfide. The expected annual number of truck accidents for the Nation was 0.18, and the expected number of years between spills was thirty-five.

TABLE 5. ESTIMATED NUMBER OF TRUCK ACCIDENTS INVOLVING PHOSPHORUS PENTASULFIDE, BY STATE, 1987

State	Estimated Accidents†	Estimated Years/Spill†
Alabama	0.01	833
Arkansas	0.01	833
Delaware	0.00	6,667
Illinois	0.01	1,111
Indiana	0.00	3,333
Kansas	0.00	1,667
Louisiana	0.01	606
Maryland	0.00	6,667
Mississippi	0.03	202
Missouri	0.01	667
New Jersey	0.01	952
Ohio	0.02	444
Oklahoma	0.03	196
Pennsylvania	0.02	278
Tennessee	0.00	2,222
Texas	0.02	290
U.S.	0.18	35

†The number of highway accidents is calculated at one accident per one million truck-miles. Truck-miles are reported in Table 4. About 15 percent of these accidents results in a release or spill. These rules of thumb were suggested by RSPA's Office of Hazardous Materials Safety.

Data from the U.S. DOT hazardous materials database were examined to determine if these results were consistent with actual experience for the years 1985 through 1992. Only three reported phosphorus pentasulfide incidents were found. These data are shown in Table 6. Two of the incidents were caused by packaging failure, and one was caused by human error. None is attributable to a highway accident. This is not surprising, given that only 0.18 accidents are expected in any given year (or 1.44 accidents over an eight-year period). The incident involving human error was a negligible spill for a less-than-truck-load shipment to a pharmaceutical company. This type of shipment is not within the scope of this study, which focuses on large-volume shipments.

TABLE 6. DATA ON PHOSPHORUS PENTASULFIDE INCIDENTS FROM U.S. DOT HAZMAT DATABASE 1985 TO 1992

Origin State	Destination State	Spill State	Release Amount (Pounds)	Cause†	Type of Consignee‡
IL	NJ	OH	1,500	20	Chemical
KS	LA	MO	930	20	Unknown
PA	NC	PA	negligible	10	Pharmaceutical

†Cause of release: 10 denotes human error; 20 denotes packaging failure; 30 denotes highway accident; and 40 denotes all other.

‡Chemical denotes a chemical manufacturer or wholesaler; pharmaceutical denotes a pharmaceutical company; and unknown indicates that the company name was not given, although the location of the consignee was given, and that location was consistent with a major chemical company.

Source: U.S. Department of Transportation

The other two incidents likely involved large volume shipments. Release amounts were 930 and 1,500 pounds, and these occurred in Missouri and Ohio, respectively, states with above average ton-miles of phosphorus pentasulfide moving by highway.

APPENDIX A. LIST OF 147 LARGE-VOLUME CHEMICALS

Chemical	Production Volume, 1987 (Thousands of Short Tons)
Sulfuric Acid	39,235
Propane	26,896
Nitrogen	24,515
Oxygen	16,669
Ammonia	16,100
Calcium Oxide	15,733
Sodium Hydroxide	11,486
Chlorine Gas	11,019
Phosphoric Acid	10,685
Sulfur	10,321
Carbon Dioxide	8,307
Ethylene Dichloride	7,878
Ammonium Nitrate	7,612
Nitric Acid (100% HNO3 Basis)	7,225
Benzene	5,904
Ethylbenzene	4,630
Vinyl Chloride	4,201
Styrene	4,007
Methanol	3,769
Toluene	3,223
Ethylene Oxide	2,921
Hydrochloric Acid (100%)	2,869
p-Xylene	2,578
Methyl t-Butyl Ether	1,757
Phenol	1,676
Acetic Acid, Synthetic	1,623
1,3-Butadiene	1,465
Ethanol (Synthetic)	1,434
Aluminum Sulfate	1,426
Carbon Black (Furnace Black)	1,362
Vinyl Acetate	1,253
Acrylonitrile	1,250
Formaldehyde	1,232
Cyclohexane	1,137
Propylene Oxide	1,105

APPENDIX A. LIST OF 147 LARGE-VOLUME CHEMICALS, (Continued)

Chemical	Production Volume, 1987 (Thousands of Short Tons)
Acetone	1,048
Butyraldehyde	879
Acetic Anhydride	858
Adipic Acid	795
Isopropanol	685
Nitrobenzene	625
1-Butanol	575
Argon	560
Acrylic Acid	550
Hexamethylenediamine	543
Isobutylene	518
Hydrogen Cyanide	516
Methyl Methacrylate	514
Phthalic Anhydride	508
o-Xylene	470
Methylene Diphenyl Diisocyanate	467
Cyclohexanone	465
Barite	448
Aniline	430
Hexane	426
Phosgene	421
Linear Alkylate Sulfonate	399
Hydrogen	389
Carbon Tetrachloride	374
Acetaldehyde	363
Toluene Diisocyanate	357
Methylchloroform	347
Phosphorus	344
Methyl Ethyl Ketone	336
Sodium Chlorate	289
Tripropylene (Nonene)	275
Hydrofluoric Acid	274
Methyl Chloride	261
Methylene Dichloride	259
n-Butyl Acrylate	258

APPENDIX A. LIST OF 147 LARGE-VOLUME CHEMICALS, (Continued)

Chemical	Production Volume, 1987 (Thousands of Short Tons)
Potassium Hydroxide	246
Perchloroethylene	237
1-Butene	231
Calcium Carbide	230
Sulfur Dioxide	229
Epichlorohydrin	225
Chloroform	224
Dodecene (Propylene Tetramer)	200
Maleic Anhydride	193
Dichlorodifluoromethane (F12)	184
Acetylene	182
Carbon Disulfide	180
Ethylene Glycol Monobutyl Ether	175
Bromine	168
Ethyl Acrylate	162
Hydrogen Peroxide	153
Chlorodifluoromethane (F22)	142
n-Pentane	142
Propionaldehyde	140
Ferric Chloride	137
Nonylphenol	137
Sodium Chromate/Dichromate	128
Chlorobenzene	123
Naphthalene	121
Monoethanolamine	116
Activated Carbon	109
Ethyl Acetate	107
Phosphorus Trichloride	102
n-Butyl Acetate	101
Isobutyraldehyde	99
Trichloroethylene	98
n-Propanol	93
Barium Sulfide	92
n-Heptane	89
Calcium Hypochlorite	88

Chemical	Production Volume, 1987 (Thousands of Short Tons)
Sodium Cyanide	85
Isobutanol	83
Pinene	78
Sodium Hydrosulfite	78
Ethyl Chloride	77
Tetrahydrofuran	77
Methyl Isobutyl Ketone	76
Chloronitrobenzene	73
Sodium (Metal)	72
Phosphorus Pentasulfide	70
Hexene-1	61
Propionic Acid	59
Acrylamide	56
Chlorinated Isocyanurates	55
Isoprene	54
Zinc Sulfate	54
Ethylene Glycol Monoethyl Ether	53
p-Dichlorobenzene	52
Dicyclopentadiene	50
Hydrofluosilicic Acid	50
Benzoic Acid	48
Isobutyl Acetate	44
Atrazine	43
Ethylene Glycol Monoethyl Ether Acetate	42
Ethylenediamine Tetraacetic Acid	41
Furfural	40
Sodium Hydrosulfide	40
Ethylenediamine	39
Dimethylamine	37
Cupric Sulfate	36
Ethylene Glycol Monomethyl Ether	36
n-Propyl Acetate	35
Aluminum Chloride	33
Benzyl Chloride	33
Phosphorus Oxychloride	31

APPENDIX A. LIST OF 147 LARGE-VOLUME CHEMICALS, (Concluded)

Chemical	Production Volume, 1987 (Thousands of Short Tons)
Ethylene Dibromide	30
Zinc Chloride	28
Isopropyl Acetate	27
Isopropylamine, Mono	27
Methylamine	26
Sodium Phosphate, Tribasic	26
Amyl Alcohol	25
Total for 147 Chemicals	288,792

APPENDIX B. MODELING TRUCK FLOWS

Models are used to allocate truck flows from the various producing plants and terminals to consuming plants that receive shipments by truck. The models are designed to estimate most likely origin-destination pairs based on a variety of considerations, as described below:

(1) The shorter the distance between an origin-destination pair, the greater the likely cargo flow between them.

(2) The larger the production or consumption of the chemical at the origin or destination, the greater the cargo flow.

(3) Corporate affiliations are sufficiently strong so that if a producing and a consuming plant are both owned by the same company, the effective distance between them is treated as equivalent to one-third the actual distance.

(4) Minimum shipment volumes of approximately 20 short tons per year are set for any given origin-destination pair. This amount is approximately equal to the minimum requirement for inclusions in the U.S. DOT's Hazardous Materials Registration Program.

(5) Available supply at each origin is set equal to the net production available for truck shipments.

(6) The total amount supplied to each destination is set equal to its estimated net product requirement specified for truck delivery.

The models start with a set of plants producing or having available for off-site shipments varying estimated quantities of the hazardous chemical under study. The quantities are typically measured in thousands of short tons per year, as listed previously in Table 2. Similarly, there are consuming plants buying or receiving estimated amounts of the chemical.

The models estimate the quantities of chemicals, termed flows, moving from the producing plants to the consuming plants. The flows can be arrayed in a two-dimensional table (see Table B-1).

TABLE B-1. PRODUCTION/CONSUMPTION FLOW MATRIX

Consumers Producers	Consumer 1	Consumer 2	Consumer 3	Total Available for Off Site Shipments
Producer 1	F_{11}	F_{12}	F_{13}	Production 1 $\geq \sum_j F_{1j}$
Producer 2	F_{21}	F_{22}	F_{23}	Production 2 $\geq \sum_j F_{2j}$
Producer 3	F_{31}	F_{32}	F_{33}	Production 3 $\geq \sum_j F_{3j}$
Producer 4	F_{41}	F_{42}	F_{43}	Production 4 $> \sum_j F_{4j}$
Total Consumption Received by	Consumption 1 $\sum_i F_{i1}$	Consumption 2 $\sum_i F_{i2}$	Consumption 3 $\sum_i F_{i3}$	Total Shipped by Truck

The F's in the table indicate the flows to be estimated. For example, F_{21} indicates the flow from producing plant 2 to consuming plant 1. Note that if we sum the flows vertically, they will equal the consumption listed across the bottom of the table. In general, however, the horizontal sums will be less than or equal to the production quantities listed at the right, because some of the production will be used for other purposes or may travel by a mode other than truck.

Based on previous research, two models are used to estimate truck flows by state.[5] These models are described below.

Gravity Model

Gravity models provide a method for filling in the above table. They are widely applied and accepted models for freight allocation problems and have been shown to be reasonable predictors of freight movements.[6] They take their name from the mathematical form, which is analogous to Newton's Law of Universal Gravitation, but otherwise they have nothing to do with gravity.

Unless they are programmed otherwise, gravity models assign the largest commodity flows to those origin-destination pairs that (a) are closest in distance and (b) have the largest volumes of product available at the origin or demanded at the destination. Gravity models also provide a routing over the actual highway network for these flows. By their mathematical structure, they tend to assign flows in such a way that all of the F_{ij}'s are non-zero, although some may be quite small. Because, in reality, companies tend to buy in large quantities, such as truckloads, the model is modified to restrict the F_{ij}'s to be at least 11 short tons. Other adjustments, such as giving preferences to flows between producers and consumers owned by the same parent company, are incorporated into the model.

Linear Programming Model

Linear programming is the second model used for estimating the F_{ij}'s.[7] This particular application of linear programming models is part of the "Transportation Problem" in which the model tries to minimize ton-miles, truck-miles, or some other measure of transportation cost. The same input variables used in the gravity model are required for the linear programming model: information on production available for off-site consumption, demand for truck shipments by consumers, and estimated miles between each producer and consumer.

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[5] "Alternative Modeling Approaches for Allocating Truck Flows of Hazardous Chemicals," a draft report prepared for RSPA's Office of Hazardous Materials Safety by the RSPA/Volpe Center and TDS Economics, July 1994.

[6] K. Rask Overgaard, "Traffic Estimating and Planning," *Acta Polytechnica Scandinavica*, Civil Engineering and Building Construction Series No. 37, 1966.

[7] N. Kwak, *Mathematical Programming with Business Applications*, McGraw-Hill, Inc., 1973.

The linear programming approach, however, is quite different from the gravity model approach in several respects. The linear programming model starts with an objective function, typically to minimize ton-miles or truck-miles traveled:

$$\text{Min} \sum_{ij} F_{ij}.$$

This model is ideally suited for the decision process of a single company interested in minimizing its transportation costs. It may be less applicable to modeling the decisions of multiple companies that are not all working together to minimize total industry-wide transportation costs.

Due to the mathematical nature of linear programming models, flows are assigned to only a few F_{ij}'s; many of the F_{ij}'s are zero. The same constraints as those used by gravity models on the flows--for example, adjustments to favor flows between producers and consumers owned by the same company--are incorporated into the model to reflect the realities of the transportation decision making process.

Model Comparison

The two model types, gravity and linear programming, provide alternative methods for analyzing truck flows. The first tends to assign flows to most possible origin-destination pairs, while the other assigns flows to only a few pairs. The results of the two approaches show the range of possible outcomes, which are subject to many factors beyond simple mathematical modeling, such as fuel prices, corporate alliances, and the desire of purchasing companies to have multiple sources of supply.

APPENDIX C. GRAVITY MODEL ESTIMATES OF BULK SHIPMENTS OF PHOSPHORUS PENTASULFIDE BY STATE

This appendix reports the gravity model estimates of bulk shipments of phosphorus pentasulfide and compares them with the estimates of the linear programming model presented in the main body of the text. The gravity model results are shown in Table C-1. Gravity models tend to identify more connections between producer and consumer plants than do linear programming models. For this reason, the gravity model results for phosphorus pentasulfide identify flows in four states that are not included in the linear programming results: Georgia, Kentucky, Virginia, and West Virginia.

Of the estimated 12 million ton-miles of phosphorus pentasulfide moved by truck in 1987, over 17 percent occurred in Missouri, a state with two plants that receive shipments of this chemical. Mississippi, with almost 13 percent of the ton-miles, has neither producing nor consuming plants. Pennsylvania, with over 11 percent of the total ton-miles, has a production plant in Morrisville, and Ohio, with slightly under 10 percent of the total ton-miles, has receiving plants in Hooven and Painesville.

The gravity model results shown in Table C-1 are reflected on the maps in Figures 3 and 4, which show the major routes carrying truck shipments of phosphorus pentasulfide.[8] The width of the blue lines is directly proportional to the quantity flowing over the routes, as indicated in the figure legends. The direction of flow is indicated by the position of the flow line relative to its route, shown in red. A blue flow line shown to the right of a north-south route indicates that the flow is northward. A blue flow line that lies above an east-west route line indicates that the flow is westward.

The national map, shown in Figure 3, indicates that there are no truck shipments of phosphorus pentasulfide west of Kansas, Oklahoma, and Texas. As shown in Figures 3 and 4, the gravity model indicates that there are four major and several minor routes. First, there are two major flows from the Monsanto plant in Sauget, Illinois. One major flow moves south through Missouri, Arkansas, Mississippi, and Louisiana to Port Arthur, Texas and Belle Chasse, Louisiana. The second major flow from Sauget moves east through Indiana and Ohio to the Lubrizol plant in Painesville. Also, there are two major flows from the Rhone-Poulenc plant in Morrisville, Pennsylvania. One route carries the chemical northwest to Painesville; the other carries phosphorus pentasulfide eastward to the American Cyanamid plant in Linden, New Jersey. As explained on page 6, the gravity model may well have identified some flows of phosphorus pentasulfide that do not in fact exist.

[8]The software used to generate the flow maps is described in Appendix D.

TABLE C-1. GRAVITY MODEL ESTIMATES OF BULK TRUCK SHIPMENTS OF PHOSPHORUS PENTASULFIDE BY STATE, 1987

State	Ton-miles (Thousands)	Truck-miles (Thousands)†
Alabama	440	16
Arkansas	342	12
Delaware	36	1
Georgia	20	1
Illinois	791	29
Indiana	586	21
Kansas	657	24
Kentucky	40	1
Louisiana	933	34
Maryland	143	5
Mississippi	1,541	56
Missouri	2,095	76
New Jersey	196	7
Ohio	1,176	43
Oklahoma	326	12
Pennsylvania	1,356	49
Tennessee	325	12
Texas	618	22
Virginia	360	13
West Virginia	2	0
Total	11,983	436

†The short tons per vehicle range from 15 to 40, including both flat beds and containers. Truck-miles are calculated by dividing ton-miles by 27.5, the mid-point of this range.

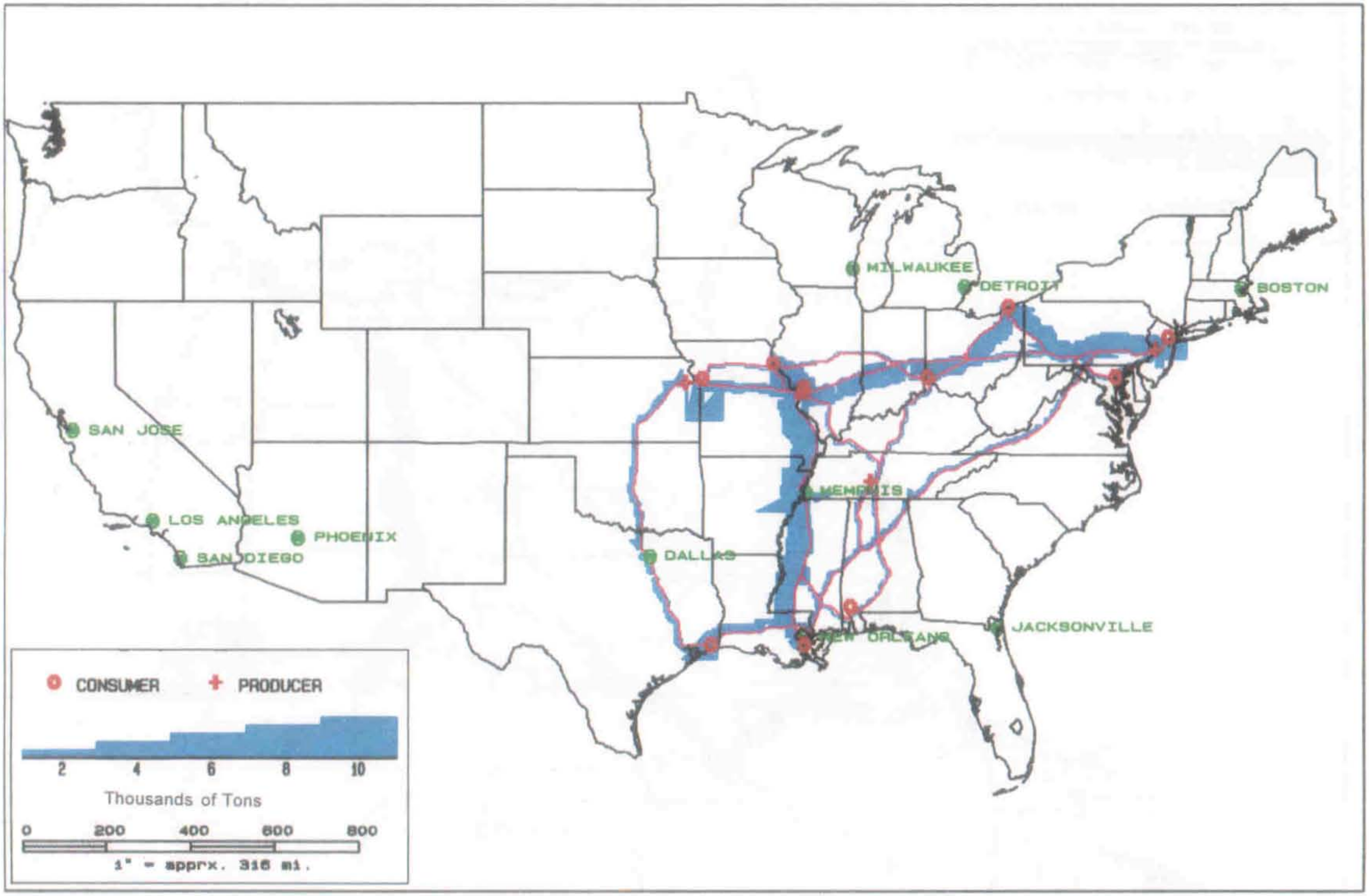

FIGURE 3. NATIONAL TRUCK FLOWS OF PHOSPHORUS PENTASULFIDE
(GRAVITY MODEL RESULTS)

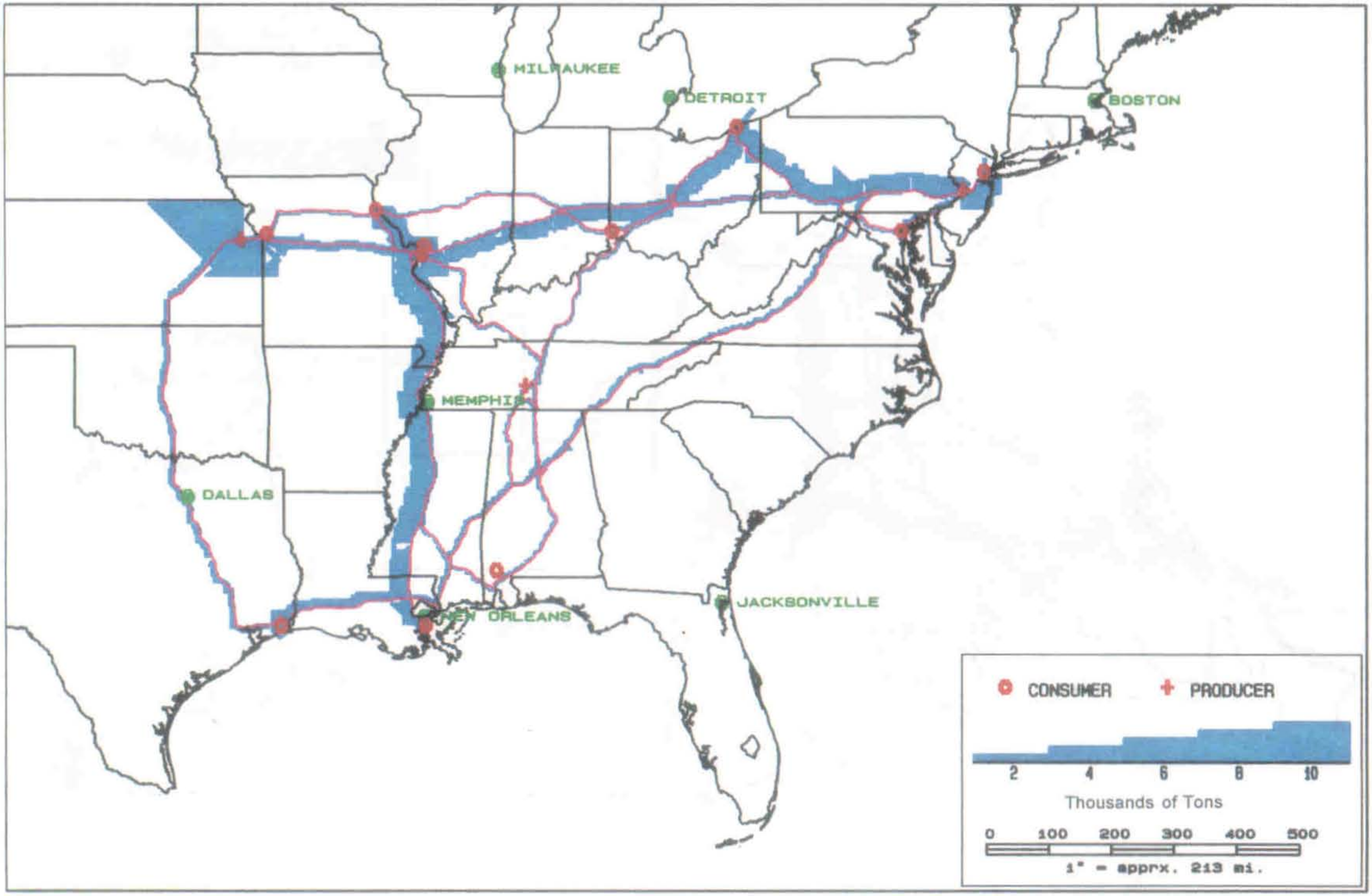

FIGURE 4. NATIONAL TRUCK FLOWS OF PHOSPHORUS PENTASULFIDE: EASTERN U.S.
(GRAVITY MODEL RESULTS)

APPENDIX D. TRANSCAD© MAP DISPLAY PROGRAM

TransCAD© mapping software, developed by the Caliper Corporation of Newton, MA, was used to prepare the maps in this report, which depict the results of the gravity and linear programming results. The software enables users to construct national, regional, and local maps on IBM-compatible personal computers. Three kinds of input data are used to produce the maps: point (node), link (flow), and area files. For this study, point and link data are used. TransCAD© input data files are the output files from the gravity and linear programming models described in Appendix B. The point data file provides the ZIP code location and descriptors for each of the producing and consuming plants. The link file provides the estimated flow (tonnage) of chemicals moving from each producing plant to each consuming plant.

TransCAD© has an auxiliary database that contains descriptors of each of the nation's roads and highways. The descriptors include such items as local, state, or federal control; paved or unpaved; all year or seasonal operating conditions; and height or weight restrictions on vehicular traffic. The software can be modified to ensure that hazardous chemicals are not moved on certain types of roads, including restricted, unpaved or seasonal roads. It tends to select larger, interstate routes and de-selects smaller, winding roads, although the model is not prevented from selecting such roads.